

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060823\
 Data File : VX036074.D
 Acq On : 08 Jun 2023 16:42
 Operator : JC/MD
 Sample : 03097-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EZER3

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
 Title : VOC Analysis

Signal : TIC: VX036074.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	15	rVB	8731	9716	0.74%	0.100%
2	1.264	26	29	32	rBV2	1308	1646	0.13%	0.017%
3	1.368	42	46	62	rVB	131490	161712	12.40%	1.659%
4	1.672	91	96	111	rBV	96371	152681	11.70%	1.566%
5	2.306	194	200	210	rBV	278477	432265	33.14%	4.435%
6	2.404	211	216	230	rVB	5336	16174	1.24%	0.166%
7	2.495	230	231	232	rBV	318	178	0.01%	0.002%
8	2.611	249	250	252	rVV	349	147	0.01%	0.002%
9	2.648	255	256	259	rBV2	338	285	0.02%	0.003%
10	2.733	268	270	273	rBV2	258	289	0.02%	0.003%
11	2.782	276	278	279	rBV2	993	694	0.05%	0.007%
12	2.886	293	295	296	rBV	283	173	0.01%	0.002%
13	3.386	376	377	380	rVB	279	188	0.01%	0.002%
14	3.520	396	399	400	rVB	292	187	0.01%	0.002%
15	3.562	400	406	411	rBV3	239	401	0.03%	0.004%
16	3.623	415	416	418	rBV3	264	226	0.02%	0.002%
17	3.733	432	434	437	rVB	313	335	0.03%	0.003%
18	3.776	437	441	444	rBV2	311	470	0.04%	0.005%
19	3.904	460	462	465	rVB2	176	151	0.01%	0.002%
20	3.989	474	476	479	rVV2	220	209	0.02%	0.002%
21	4.129	498	499	502	rBV	185	155	0.01%	0.002%
22	4.190	507	509	510	rBV	229	191	0.01%	0.002%
23	4.471	545	555	570	rBV	78667	268525	20.58%	2.755%
24	4.910	625	627	629	rBV2	245	210	0.02%	0.002%
25	5.056	639	651	671	rBV	162807	517811	39.69%	5.312%
26	5.330	694	696	698	rBV2	221	153	0.01%	0.002%
27	5.385	701	705	710	rVV2	730	1427	0.11%	0.015%
28	5.550	725	732	742	rVB4	1539	4386	0.34%	0.045%
29	5.745	762	764	766	rBV2	207	234	0.02%	0.002%
30	5.861	781	783	786	rVB	229	175	0.01%	0.002%
31	5.970	789	801	820	rBV2	439462	1304506	100.00%	13.383%
32	6.281	848	852	853	rBV2	271	265	0.02%	0.003%
33	6.415	868	874	877	rBV2	258	516	0.04%	0.005%
34	6.757	921	930	945	rBV	323679	781298	59.89%	8.015%
35	7.117	982	989	994	rBV5	1162	2759	0.21%	0.028%
36	7.208	1002	1004	1007	rVB2	213	216	0.02%	0.002%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
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37	7.306	1012	1020	1034	rBV	271431	599749	45.98%	6.153%
38	7.476	1044	1048	1053	rBV3	881	1326	0.10%	0.014%
39	7.586	1065	1066	1068	rBV2	262	217	0.02%	0.002%
40	7.775	1095	1097	1099	rBV2	257	215	0.02%	0.002%
41	7.830	1104	1106	1109	rVV	308	199	0.02%	0.002%
42	7.903	1114	1118	1119	rBV2	804	1032	0.08%	0.011%
43	8.226	1167	1171	1172	rBV	134	205	0.02%	0.002%
44	8.324	1179	1187	1202	rBV	170882	274845	21.07%	2.820%
45	8.586	1226	1230	1233	rBV2	328	405	0.03%	0.004%
46	8.647	1233	1240	1249	rBV	668197	1033300	79.21%	10.601%
47	8.872	1273	1277	1278	rVB2	251	287	0.02%	0.003%
48	8.952	1283	1290	1300	rBV	118596	182247	13.97%	1.870%
49	9.061	1307	1308	1311	rVB2	398	352	0.03%	0.004%
50	9.238	1336	1337	1338	rBV	238	152	0.01%	0.002%
51	9.269	1340	1342	1348	rVB3	927	1267	0.10%	0.013%
52	9.384	1355	1361	1374	rBV	424672	597857	45.83%	6.133%
53	9.598	1393	1396	1397	rBV	385	398	0.03%	0.004%
54	9.732	1416	1418	1420	rBV	225	165	0.01%	0.002%
55	9.756	1420	1422	1426	rVB2	301	332	0.03%	0.003%
56	10.055	1465	1471	1481	rBV	658816	921305	70.62%	9.452%
57	10.238	1500	1501	1503	rVB2	341	154	0.01%	0.002%
58	10.305	1506	1512	1515	rBV5	1665	2395	0.18%	0.025%
59	10.439	1529	1534	1537	rBV2	310	677	0.05%	0.007%
60	10.640	1565	1567	1569	rBV2	452	404	0.03%	0.004%
61	10.774	1587	1589	1590	rBV2	399	325	0.02%	0.003%
62	11.024	1628	1630	1632	rVB2	237	161	0.01%	0.002%
63	11.043	1632	1633	1636	rVB	242	181	0.01%	0.002%
64	11.085	1637	1640	1646	rVB3	878	1221	0.09%	0.013%
65	11.189	1652	1657	1666	rVB	469057	587792	45.06%	6.030%
66	11.421	1692	1695	1699	rVV2	808	866	0.07%	0.009%
67	11.451	1699	1700	1703	rVV	337	262	0.02%	0.003%
68	11.646	1729	1732	1734	rBV2	150	147	0.01%	0.002%
69	11.713	1740	1743	1744	rVB	582	489	0.04%	0.005%
70	11.963	1782	1784	1786	rVB	265	139	0.01%	0.001%
71	12.018	1788	1793	1802	rVV	693442	868948	66.61%	8.914%
72	12.219	1821	1826	1837	rVV	68672	115568	8.86%	1.186%
73	12.317	1837	1842	1852	rVB	700621	878682	67.36%	9.014%
74	12.926	1941	1942	1944	rBV2	329	192	0.01%	0.002%
75	13.030	1956	1959	1960	rBV	377	356	0.03%	0.004%
76	13.207	1986	1988	1991	rBV2	368	356	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

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Peak Location: TOP

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 Title : VOC Analysis

77	13.268	1997	1998	2001	rBV3	526	493	0.04%	0.005%
78	13.408	2019	2021	2024	rBV2	295	360	0.03%	0.004%
79	13.524	2037	2040	2042	rBV2	283	404	0.03%	0.004%
80	13.689	2063	2067	2070	rBV3	680	1052	0.08%	0.011%
81	13.774	2079	2081	2087	rVB2	958	898	0.07%	0.009%
82	13.908	2101	2103	2104	rBV2	362	226	0.02%	0.002%
83	13.945	2108	2109	2113	rVB2	387	360	0.03%	0.004%
84	14.018	2117	2121	2123	rBV2	278	371	0.03%	0.004%
85	14.121	2133	2138	2142	rBV3	962	1532	0.12%	0.016%
86	14.225	2154	2155	2158	rVB2	383	195	0.01%	0.002%
87	14.292	2165	2166	2169	rVB2	355	257	0.02%	0.003%
88	14.432	2187	2189	2190	rBV	326	169	0.01%	0.002%
89	14.451	2190	2192	2195	rBV3	621	722	0.06%	0.007%
90	14.566	2209	2211	2213	rBV2	393	391	0.03%	0.004%
91	14.634	2220	2222	2224	rVB2	675	514	0.04%	0.005%
92	14.853	2257	2258	2259	rBV	376	202	0.02%	0.002%
93	15.359	2339	2341	2343	rBV2	575	360	0.03%	0.004%
94	15.542	2369	2371	2372	rBV	847	449	0.03%	0.005%
95	15.737	2401	2403	2406	rBV3	556	525	0.04%	0.005%
96	15.938	2434	2436	2439	rBV2	483	596	0.05%	0.006%
97	16.152	2469	2471	2472	rVB	497	288	0.02%	0.003%
98	16.261	2488	2489	2491	rBV2	540	311	0.02%	0.003%
99	16.347	2501	2503	2505	rBV2	413	306	0.02%	0.003%
100	16.371	2505	2507	2510	rVB2	527	517	0.04%	0.005%

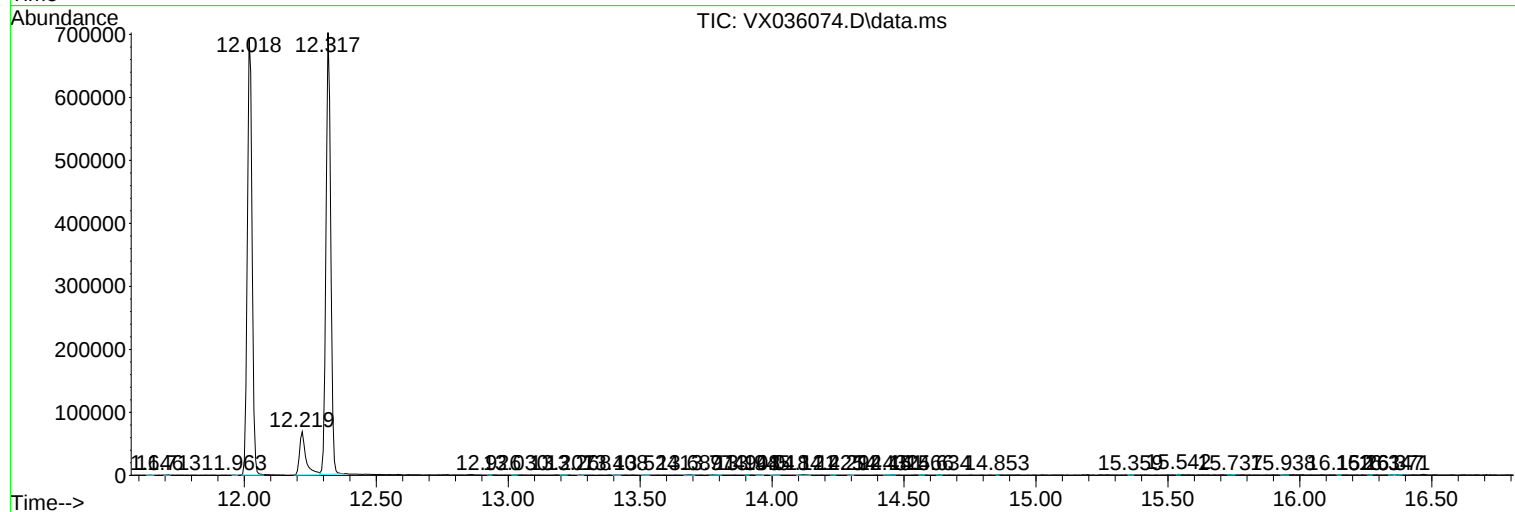
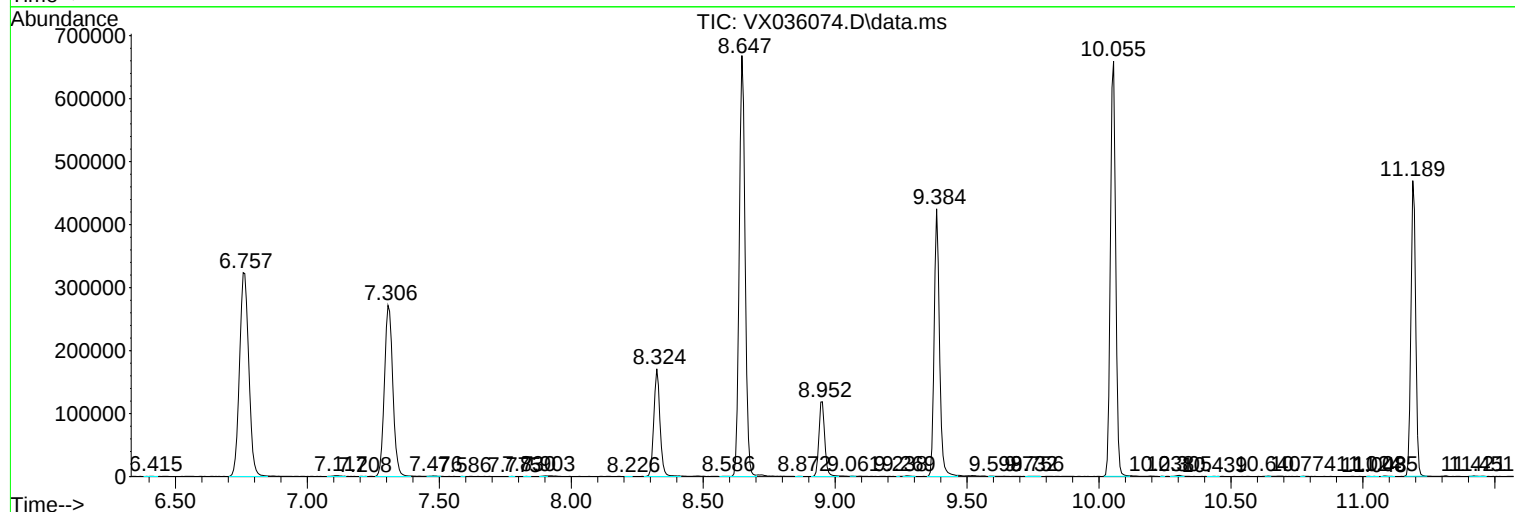
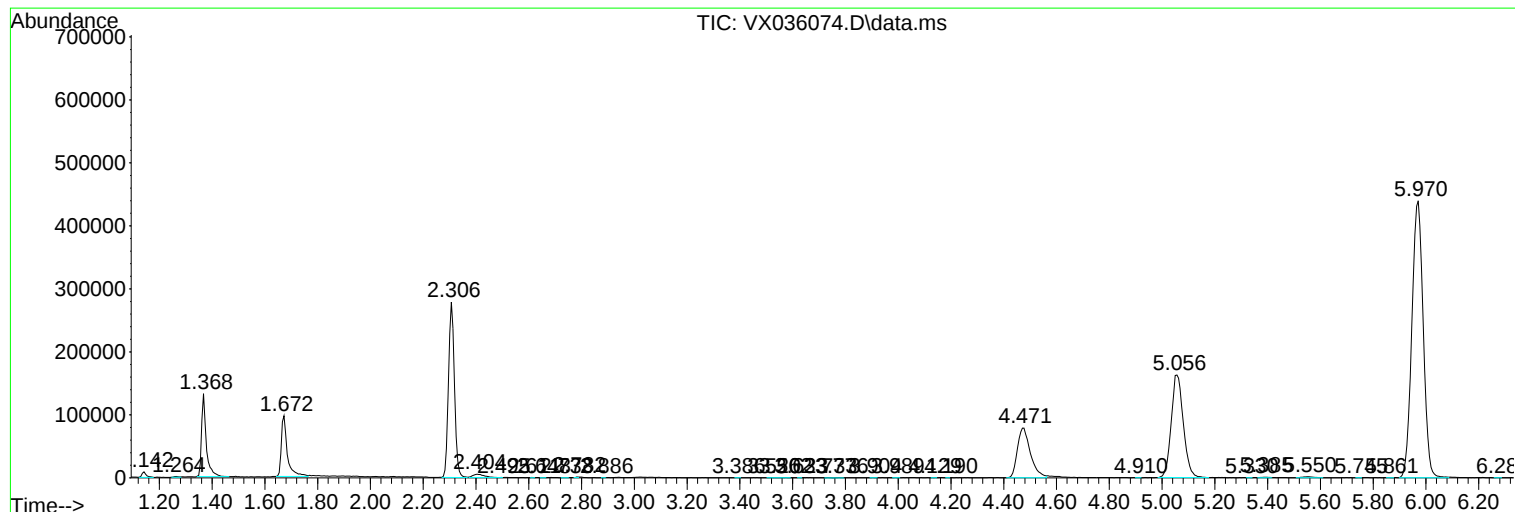
Sum of corrected areas: 9747622

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EZER3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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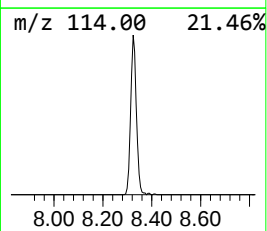
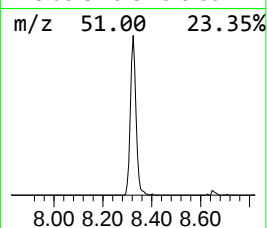
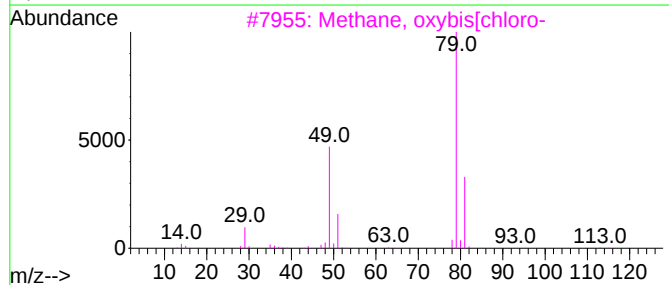
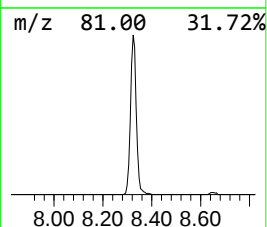
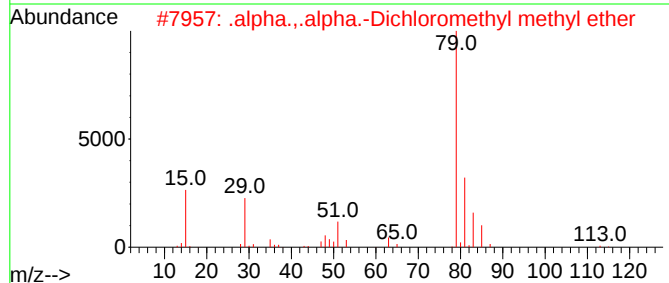
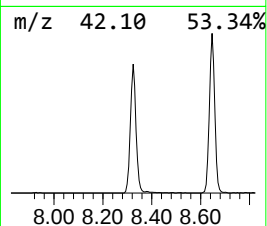
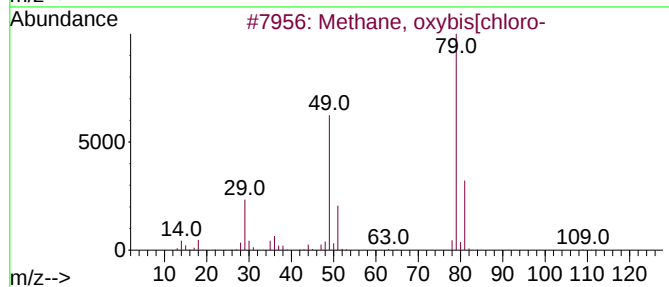
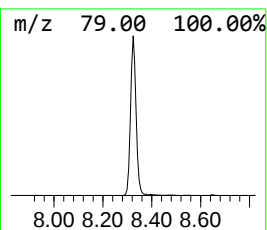
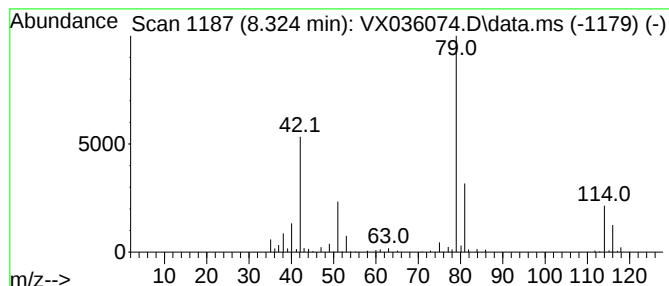
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.324	17.59 ug/L	274845	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	25
2			.alpha.,.alpha.-Dichloromethyl m...	114	C2H4Cl2O	004885-02-3	25
3			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	23
4			2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	17
5			Thiophosgene	114	CCl2S	000463-71-8	10



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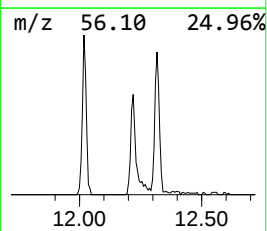
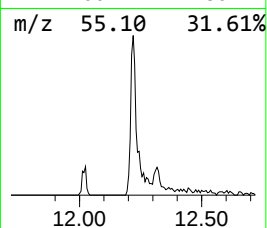
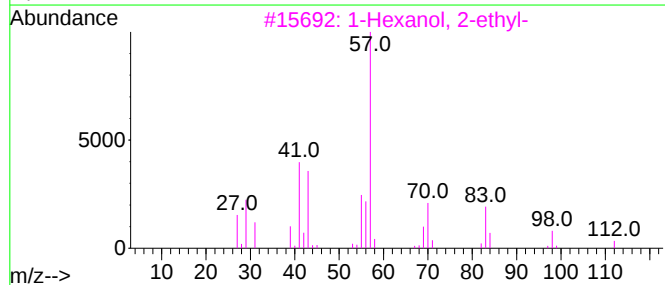
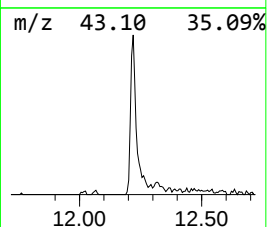
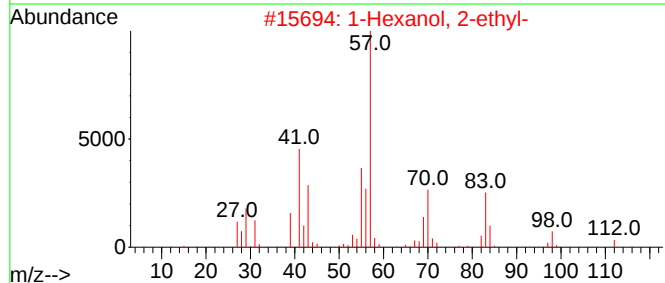
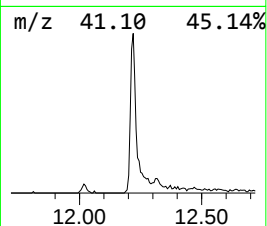
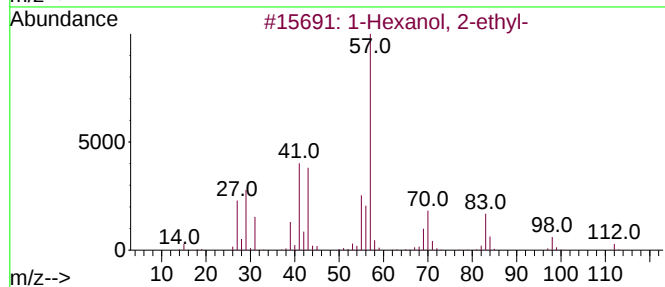
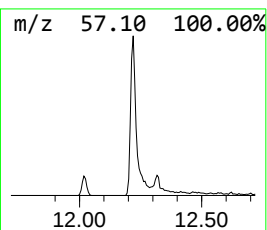
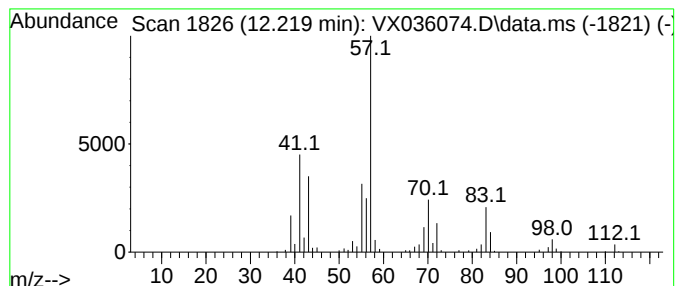
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	6.65 ug/L	115568	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	86
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59



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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	8.324	17.6	ug/L	274845	1	6.757	781298	50.0
1-Hexanol, 2-et...	12.219	6.7	ug/L	115568	3	12.024	868948	50.0